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Superconducting state parameters of metals

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Abstract : The theoretical investigation of five superconducting state parameters (SSP) *viz.* electron–phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_C, isotope effective exponent α and interaction strength N_OV of five monovalent (Li, Na, K, Rb and Cs), two divalent (Mg and Zn) and five polyvalent (In, Tl, Sn, Pb and Bi) metals have been carried out by our well-recognized and recently proposed model pseudopotential. We have employed here five different types of local field correction functions proposed by Hartree, Taylor, Ichimaru-Utsumi, Farid *et al* and Sarkar *et al* to study the exchange and correlation effects on the present computations. The recent local field correction functions due to Ichimaru-Utsumi, Farid *et al* and Sarkar *et al* have been employed for the first time in the study of SSP of metals. A very strong influence of all the exchange and correlation functions is found in the present study. Our results are in fair agreement with other available theoretical as well as experimental data. A strong dependency of the SSP of metals on the valency Z is found.

Keywords : Pseudopotential, superconducting state parameters.

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1. Introduction

During last several years, the superconductivity remains a dynamic area of research in condensed matter physics with continual discoveries of novel materials and with an increasing demand for novel devices for sophisticated technological applications. A large number of metals and alloys are superconductors, with critical temperature T_c ranging from 1–18 K. Even some heavily doped semiconductors have also been found to be superconductors. Basically all the metal superconductors are type-I superconductors at room temperature [1,2]. The pseudopotential theory has been used successfully in explaining the superconducting state parameters (SSP) for metals by many workers [3–15]. Many of them have used Sharma-Kachhava's linear potential [16] as well as Ashcroft's empty core model potential [17] in the calculation of SSP for metals. Recently, we have calculated the SSP for some binary alloys and metallic glasses [18, 19] based on the model potential formalism.

In the present study, we have used McMillan's theory [14] and our model potential formulation [20,21] for predicting the SSP in five monovalent (Li, Na, K, Rb and Cs), two divalent (Mg and Zn) and five polyvalent (In, Tl, Sn, Pb and Bi) metals. We have used our well-recognized model potential [20,21] for studying electron–phonon coupling strength λ, Coulomb pseudopotential μ^*, transition temperature T_c, isotope effect exponent α and effective interaction strength N_OV. To see the impact of various exchange and correlation functions on the aforesaid properties, we have used five different types of local field correction functions proposed by Hartree (H) [22], Taylor (T) [23], Ichimaru-Utsumi (IU) [24], Farid *et al* (F) [25] and Sarkar *et al* (S) [26]. We have incorporated for the first time the advanced local field correction functions *i.e.* IU [24], F [25] and S [26] in the investigation of the SSP.

2. Theoretical methodology

The real-space form of the proposed model potential used to describe the electron-ion interaction is given by [20,21]

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$$V(r) = \frac{-Ze^2}{r_c^3}\left[2 - \exp\left(1 - \frac{r}{r_c}\right)\right], \quad r \le r_c$$

$$\frac{-Ze^2}{r}, \quad r \ge r_c, \tag{1}$$

Where r_c is the potential parameter. This form has feature of a Coulombic term outside the core and varying cancellation due to a repulsive and attractive contributions to the potential within the core.

The corresponding form factor in momentum space is given as [20,21]

$$V(q) = \frac{-4\pi Ze^2}{\varepsilon(q)\Omega_0 q^2}\left[-1 + \frac{12}{U^2} + \frac{U^2}{1+U^2} + \frac{6U^2}{(1+U^2)^2} + \frac{18U^4}{(1+U^2)^3} + \frac{6U^4}{(1+U^2)^3} + \frac{24U^2}{(1+U^2)^4} - \frac{24U^4}{(1+U^2)^4}\right]\cos(U)$$

$$\left[\frac{6}{U} - \frac{12}{U^3} + \frac{U}{1+U^2} + \frac{3U}{(1+U^2)^2} + \frac{3U^3}{(1+U^2)^2} + \frac{6U}{(1+U^2)^3} + \frac{18U^3}{(1+U^2)^3} + \frac{6U}{(1+U^2)^4} - \frac{36U^2}{(1+U^2)^4} + \frac{6U^4}{(1+U^2)^4} + 24U^2\exp(1)\left\{\frac{U^2-1}{(1+U^2)^4}\right\}\right]\sin(U) \tag{2}$$

Here, $U = qr_c$, r_c is the potential parameter. Z, e, Ω_0, q and $\varepsilon(q)$ are the valency, electronic charge, atomic volume, wave vector and modified Hartree dielectric function, respectively. The various forms of local field correction function [21–26] affect the potential through $\varepsilon(q)$.

The electron-phonon coupling strength λ is computed using [3-7,11–14,18,19]

$$\lambda = \frac{12m^*Z^*}{M\langle\omega^2\rangle}\int_0^1 X^3|V(X)|^2\,dX \tag{3}$$

Here, m^* is the effective electronic mass, M the ionic mass, Z^* the effective valence, $X = q/2k_F$ where k_F is the Fermi wave vector, $V(X)$ the screened pseudopotential and $\langle\omega^2\rangle$ the averaged square of phonon frequency, with $\langle\omega\rangle^{1/2} = (\omega_L + \omega_T)/2$ of the metal, respectively ω_L and ω_T are the maximum frequency of longitudinal and transverse modes of the phonon spectrum as measured by neutron scattering experiments [4–7]. For Bi, values of ω_L and ω_T are not available, so the averaged square phonon frequency $\langle\omega^2\rangle$ is calculated from the relation $\langle\omega^2\rangle^{1/2} = 0.69\,\theta_D$ [19].

The Coulomb pseudopotential μ^* is given by [11–13,18,19]

$$\mu = \frac{\frac{m_b}{\pi k_F}\int_0^1 \frac{dX}{\varepsilon(X)}}{1 + \frac{m_b}{\pi k_F}\left(\frac{E_F}{10\theta_D}\right)\int_0^1 \frac{dX}{\varepsilon(X)}} \tag{4}$$

where E_F is the Fermi energy, m_b the band mass of the electron, θ_D the Debye temperature and $\varepsilon(X)$ the modified Hartree dielectric function.

The impact of various exchange and correlation functions thus seen on λ and μ^* through screened form factor $V(X)$ and $\varepsilon(X)$, respectively.

After evaluating λ and μ^*, the transition temperature T_c and isotope effect exponent α are investigated from the McMillan's formula [3–7,11–14,18,19]

$$T_c = \frac{\theta_D}{1.45}\exp\left[\frac{-1.04(1+\lambda)}{\lambda - \mu^*(1+0.62\lambda)}\right] \tag{5}$$

$$\alpha = \frac{1}{2}\left[1 - \mu^* \ln\left(\frac{\theta_T}{1.45T_c}\right)\right]\left[\frac{1+0.62\lambda}{1.04(1+\lambda)}\right] \tag{6}$$

The effective interaction strength (N_OV) is computed using the relation [4–7,18,19]

$$N_OV = \frac{\lambda - \mu^*}{1 + \frac{10}{11}\lambda} \tag{7}$$

3. Results and discussion

The input parameters and other constants used in the present computations of the SSP of five monovalent, two divalent and five polyvalenet metals are shown in Table 1.

Table 1. The input parameters and other constants for metals.

Metal	Z	Z^*	Ω_0 (a.u)	r_c (a.u)	θ_D (K)	m_b	
Li	1	1.03	144.9	1.4543	352	1.19	2.20
Na	1	1.10	254.5	2.0231	157	1.00	1.26
K	1	1.14	481.4	2.6369	59.4	0.94	1.24
Rb	1	1.17	567.9	2.7883	54	1.00	1.25
Cs	1	1.19	745.5	3.5910	40	0.98	1.43
Mg	2	2.16	155.9	1.7136	400	1.01	1.33
Zn	2	2.20	102.0	1.3492	309	0.92	0.86
In	3	3.30	175.3	1.3902	109	0.89	1.39
Tl	3	3.42	191.7	1.3899	87	0.82	1.14
Sn	4	4.28	181.5	1.3380	195	0.93	1.29
Pb	4	4.36	203.4	1.3800	96.3	0.86	2.01
Bi	5	5.35	239.4	1.3366	119	0.87	0.87

Table 2(a) shows the comparison of presently calculated values of the SSP, of monovalent alkali metals with the other such theoretical [3,5,11,12,14,15], as well as experimental [6] results. From the study of Table 2(a) it is seen that Li should become a superconductor at very high values of T_c, but experimentally it is found that it becomes a superconductor at very low temperature. Thus for Li, the present results are not showing any remarkable agreement with other available data. The presently calculated values of all the five SSP from H-screening function [22] for Na, K, Rb and Cs metals are higher than the others. Also, it can be seen from the Table 2(a) that the Coulomb pseudopotential μ^* calculated from H-screening function [22] gives better agreement with the results reported by others in comparison with the screening

Table 2(a). Superconducting state parameters for alkali metals.

Metal	SSP	Present results IU					Expt. [6]	Others
		1.0989	1.7385	1.8708	1.9336	1.5416		0.10 [11],0.11 [3], 0.15 [11], 0.21 [5], 0.37 [15],0.45 [11],0.53 [15], 0.56 [15]
	μ^*	0.1829	0.2033	0.2062	0.2078	0.1973	–	0.16 [11], 0.17 [3], 0.17 [5], 0.18 [11]
Li	T_C(K)	15.394	27.880	29.891	30.751	24.656	<0.08	1.06×10^{-26} [5], 2.68×10^{-19} [3], 0.02 [15], 0.02 [11], 1.1 [15], 1.5 [15]
	α	0.4020	0.4294	0.4325	0.4336	0.4247	–	–
	N_0V	0.4583	0.5949	0.6164	0.6258	0.5598	–	–0.05 [3], 0.035 [5], 0.09 [3], 0.13 [11], 0.13 [11]
	λ	0.2606	0.4182	0.4519	0.4679	0.3774	–	0.12 [12], 0.15 [14],0.19 [14], 0.23 [14], 0.27 [3], 0.28 [14]
	μ^*	0.1621	0.1823	0.1853	0.1873	0.1766	–	0.16 [3],0.16 [12], 0.18 [14]
Na	T_C(K)	1.47×10^{-6}	0.0431	0.0956	0.1277	0.0136	–	1.25×10^{-12} [3]
	α	–3.317	–0.372	–0.219	–0.173	–0.584	–	–5.38 [12]
	N_0V	0.0797	0.1708	0.1890	0.1969	0.1495	–	–0.17 [12], 0.09 [3]
		0.3478	0.5844	0.6347	0.6589	0.5258		0.11 [3], 0.12 [11], 0.12[11], 0.14 [15], 0.14 [11], 0.22 [15]
	μ^*	0.1601	0.1831	0.1861	0.1883	0.1765		0.15 [15], 0.16 [3], 0.16 [11], 0.16 [5], 0.18 [11], 0.18 [11]
K	T_C(K)	0.0065	0.4501	0.6656	0.7700	0.2676	–	1.56×10^{-27} [3], 0.168 [5]
	α	–0.4306	0.1645	0.2090	0.2218	0.1147	–	–
	N_0V	0.1426	0.2621	0.2845	0.2942	0.2363	–	–0.45 [3], –0.032 [11], 0.005 [3], 0.007 [5]
	λ	0.3902	0.6760	0.7380	0.7695	0.6030	–	0.095 [11],0.12 [3], 0.14 [15]
(7)	μ^*	0.1569	0.1779	0.1805	0.1826	0.1719	–	0.11 [3],0.15 [15], 0.18 [11]
Rb	T_C(K)	0.0228	0.6073	0.8279	0.9371	0.3955	–	–
	α	–0.0788	0.2816	0.3096	0.3185	0.2484	–	–
	N_0V	0.1722	0.3085	0.3336	0.3453	0.2784	–	–0.005 [3], –0.044 [11], 0.009 [3]
	λ	0.3170	0.5922	0.6195	0.6659	0.4836	–	0.12 [15], 0.19 [15], 0.28 [15]
	μ^*	0.1540	0.1753	0.1778	0.1800	0.1687	–	–
Cs	T_C(K)	0.0009	0.2517	0.3031	0.4096	0.0805	–	5×10^{-5} [15]
	α	–0.6030	0.2202	0.2356	0.2658	0.0917	–	–
	N_0V	0.1265	0.2710	0.2826	0.3027	0.2188	–	–

Table 2(b). Superconducting state parameters for divalent metals.

Metal	SSP	Present results					Expt.	Others
		H	T	IU	F	S	[6,7]	
	λ	0.3386	0.4696	0.4862	0.4957	0.4305	–	0.16 [3], 0.23 [5], 0.31 [14], 0.31[12], 0.35 [14], 0.38 [14]
	μ^*	0.1526	0.1684	0.1706	0.1717	0.1634	–	0.16 [3], 0.16 [12], 0.18 [14]
Mg	T_C (K)	0.0326	0.6443	0.7942	0.8915	0.3552	–	2.124×10^{-64} [3], 0.02 [12], 0.08 [14]
	α	–0.3280	0.0603	0.0808	0.0928	–0.003	–	0.019 [3]
	N_OV	0.1422	0.2111	0.2189	0.2234	0.1920	–	–0.013 [12], 0.177 [3]
	λ	0.3111	0.4174	0.4342	0.4397	0.3894	–	0.27 [14], 0.34 [5], 0.38 [14], 0.41 [12], 0.42 [14], 0.46 [3]
	μ^*	0.1305	0.1424	0.1441	0.1449	0.1384	–	0.11 [12], 0.12 [14], 0.14 [3]
Zn	T_C (K)	0.0329	0.4361	0.5636	0.6051	0.2785	0.875	0.01 [14], 0.41 [3], 0.85 [12]
	α	–0.074	0.1679	0.1888	0.1933	0.1375	–	0.24 [3], 0.41 [14]
	N_OV	0.1407	0.1993	0.2080	0.2106	0.1854	0.175	0.02 [14], 0.17 [12], 0.19 [3]

Table 2(c). Superconducting state parameters for polyvalent metals.

Metal	SSP	Present results					Expt.	Others
		H	T	IU	F	S	[6,7]	
	λ	0.8029	1.0904	1.1377	1.1529	1.0164	–	0.26 [3], 0.69 [14], 0.67 [12], 0.76 [5], 0.88 [14], 0.89 [14], 1.16 [14]
	μ^*	0.1149	0.1246	0.1259	0.1266	0.1214	–	0.09 [12], 0.10 [12], 0.11 [3], 0.12 [14]
In	$T_C(K)$	3.8478	6.3834	6.7596	6.8716	5.8009	3.404	4.765×10^{-3} [3], 2.8[12], 3.4 [12], 4.0 [14]
	α	0.4534	0.4636	0.4637	0.4649	0.4624	0.45	0.449 [3], 0.47 [12]
	N_OV	0.3977	0.4850	0.4974	0.5011	0.4652	–	0.12 [3]
	λ	0.8835	1.2152	1.2728	1.2912	0.9570	–	0.71 [14], 0.72 [12], 1.07 [3], 1.07 [14]
	μ^*	0.1091	0.1187	0.1201	0.1207	0.1096	–	0.10 [12], 0.11 [14]
Tl	$T_C(K)$	3.8696	6.0891	6.4247	6.5232	4.4499	2.39	2.34 [12], 2.36 [12], 4.39 [3], 4.8 [14]
	α	0.4646	0.4719	0.4727	0.4728	0.4681	–	–
	N_OV	0.4294	0.5209	0.5344	0.5384	0.4532	0.27	0.22 [14], 0.48 [3]
	λ	0.7531	0.9989	1.0349	1.0473	0.9359	–	0.60 [14], 0.78 [14], 0.82 [12], 0.99 [14], 1.3 [3]
	μ^*	0.1208	0.1308	0.1322	0.1328	0.1273	–	0.09 [12], 0.11 [3], 0.11 [12], 0.12 [14]
Sn	$T_C(K)$	5.6720	9.5842	10.115	10.286	8.6038	3.722	3.75 [12], 6.20 [14], 7.35 [12], 15.2 [3]
	α	0.4412	0.4535	0.4546	0.4549	0.4519	0.47	0.44 [3]
	N_OV	0.3753	0.4549	0.4651	0.4685	0.4354	0.263	0.16 [12], 0.54 [3]
	λ	1.6306	2.1809	2.2638	2.2922	2.0341	–	0.66 [12], 0.84 [5], 1.06 [3], 1.11 [12], 1.12 [14],1.12 [14], 1.34 [14], 1.35 [14]
	μ^*	0.1091	0.1180	0.1193	0.1198	0.1150	–	0.1 [12], 0.11 [12], 0.12 [3], 0.12 [14]
Pb	$T_C(K)$	9.5563	11.678	11.930	12.010	11.214	7.196	5.58 [3], 6.49 [12], 7.2 [12], 7.6 [14]
	α	0.4836	0.4850	0.4852	0.4852	0.4850	0.48	0.48 [3]
	N_OV	0.6129	0.6916	0.7013	0.7044	0.6736	0.411	0.32 [3], 0.54 [14], 0.60 [12]
	λ	1.1482	1.5315	1.5904	1.6096	1.4289	–	0.264 [4], 0.67 [12], 0.84 [10]
	μ^*	0.1113	0.1204	0.1217	0.1222	0.1173	–	0.10 [11], 0.11 [4], 0.12 [10]
Bi	$T_C(K)$	7.9620	10.775	11.135	11.243	10.134	6.1	–
	α	0.4742	0.4779	0.4782	0.4783	0.4775	–	–
	N_OV	0.5073	0.5899	0.6005	0.6038	0.5705	–	–

functions of T [23], IU [24], F [25] and S [26]. Our study also concludes that as the atomic size of the metal increases, the influence of screening effect increases. The maximum effect of local field correction function is predicted in the case of Cs.

In Tables 2(b,c), the comparison of presently obtained data of SSP, with experimentally available values [6,7] and other various theoretical data [3–5,10–12,14,15], is reported for divalent and polyvalent metals. From Tables 2(b,c), we see that the present findings of λ calculated from H-screening function [22] of Mg, In and Tl and that from T-screening function [23] of Zn and Sn metals show comparable results with the available theoretical findings [4–9]. The experimental values of transition temperature T_c for metals like In, Zn, Tl, Sn, Pb and Bi are 3.404 K, 0.875 K, 2.39 K, 3.722 K, 7.196 K and 6.1 K, respectively. Our present results of T_C calculated from H-screening function [22] for In, Tl, Sn, Pb and Bi and that for Zn, F-screening function [25] show fair agreement with experimental findings. The experimental data of α for In, Sn and Pb metals are 0.45, 0.47 and 0.48, respectively. The excellent agreement with these numbers is achieved in the present investigations for the metals. The presently reported value of N_OV for Zn is calculated from F-screening function [25] and that for Tl, Sn and Pb from H-screening function [22] give the satisfactory results in comparison with the observed experimental data 0.175, 0.27, 0.263 and 0.411, respectively.

From the Tables 2(a,b,c), it is noted that for all the 12 metals, the results due to F-screening function [25] generate the higher values, while H-screening function [22] generates the lower values of the parameter under investigation. The results obtained from another three screening functions T [23], IU [24] and S [26] lie between these two screening functions.

With respect to static H-dielectric function [22], the relative influence of the four local field correction functions on λ of Li, Na, K, Rb, Cs, Mg, Zn, In, Tl, Sn, Pb and Bi metals is 40.27–75.94%, 44.79–79.55%, 51.18–89.45%, 54.54–97.21%, 52.56–110.06%, 27.14–46.37%, 25.17–41.35%, 26.60–93.59%, 8.32–46.14%, 23.69–39.07%, 24.79–40.57% and 24.45–40.19%. Such influence on μ^* is for Li 7.87–13.61%, for Na 7.89–15.44%, for K 10.24–17.61%, for Rb 9.56–16.38%, for Cs 9.55–16.88%, for Mg 7.02–12.47%, for Zn 5.99–10.98%, for In 5.64–10.15%, for Tl 0.43–10.60%, for Sn 5.39–9.95, for Pb 5.39–9.81% and for Bi 5.37–9.84%, respectively. These changes in λ and μ^* make considerable variation on T_c, α and N_OV.

The local field correction functions due to IU [24], F [25] and S [26] are able to generate consistent results regarding the SSP of five monovalent, two divalent and five polyvalent metals as those obtained for more commonly employed H [22] and T [23] functions. Thus the use of these more promising local field correction functions is established successfully in the study of SSP of metals.

According to Matthias rules [27,28], the metals having $Z < 2$ does not exhibit superconducting nature. Hence, the alkali metals are non-superconductors. This may be the reason that the SSP of alkali metals are not favourite quantities to investigate experimentally. Since these metals are not showing superconducting nature in normal laboratory condition, the experimental data on SSP for most of the alkali metals are not available for any comparison and further comments. But the comparisons of presently computed results of SSP with other theoretical data are encouraging, which confirms the applicability of our newly proposed model potential to explain the SSP. When we go from $Z = 2$ to $Z = 5$, *i.e.*, from Mg to Bi except Zn and Bi, the electron-phonon coupling strength λ increases with lattice spacing 'a'. Similar trends are also observed in the values of T_c for of all the metals, except Bi.

4. Conclusions

It is seen that for proper reproduction of experimental values of SSP, the choice of dielectric function is also an important parameter. The comparison of presently computed results with available theoretical and experimental findings is encouraging in the case of pure metals, which confirms the applicability of our model potential in explaining superconducting state parameters.

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